

# Behaviour of superconductivity energetic characteristics in electron-doped cuprates. A simple model

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A simple model to describe the energetic phase diagram of electron-doped cuprate superconductor is developed. Interband pairing operates between the UHB and the defect states created by doping and supplied by both extinguishing HB-s. Two defect subbands correspond to the  $(\pi, 0)$  and  $(\pi/2, \pi/2)$  momentum regions. Extended doping quenches the bare normal state gaps (pseudogaps). Maximal transition temperature corresponds to overlapping bands ensemble intersected by the chemical potential. Illustrative results for  $T_c$ , pseudo- and superconducting gaps are calculated on the whole doping scale. Major characteristics features on the phase diagram are reproduced. Anticipated manifestation of gaps doping dynamics is discussed.

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## 1 Introduction

Electron-doped high-temperature cuprate superconductors are represented by materials like  $A_{2-x}Ce_xCuO_4$  with  $A = La; Nd; Pa; Sm; Eu$ . These systems have been investigated [1-7] not so widely as the hole-doped counterparts of them. In both cases the doping process does not only metallizes the basic compound but prepares also a modified playground for the realization of the superconductivity. The electron spectrum of such strongly correlated systems is nonrigid under doping. This leads to the reconstruction of the Fermi surface or its fragments [8-11]. The investigation of electron-doped materials is essential for covering the whole active part of the energetic spectrum of a cuprate superconductor. It originates from the spectrum of a half-filled

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charge-transfer insulator and undergoes remarkable reorganization due to doping. In the case of hole doping the region near the top of the mainly oxygen band between the splitted Cu Hubbard components participates essentially in the superconductivity. In the case of electron doping the Hubbard structure is expected to be immediately encompassed with essential events near the bottom of the upper Hubbard band (UHB). For both types of doped cuprates a "defect band" near the Fermi level is created under the perturbation exerted by the introduced extra carriers [8-11]. For hole doping this new band borrows near the top of the oxygen band (citations in [12,13]). Extended doping brings it into overlap with the itinerant oxygen band [13]. A phase separation appears [14] which reorganizes the crystalline background in hole-rich and hole-poor (defect and itinerant correspondingly) regions. In the case of electron doping the defect band will be built up under the bottom of the UHB [11], see also the theoretical papers [15-18]. A phase separation seemingly does not accompany the collapse of the Hubbard band spectrum with extended doping. Both components of the latter donate the states to built up the new band in this process.

The most remarkable difference between electron- and hole doped cuprate superconductors consists in the essentially wider antiferromagnetic (AF) region in the former case. It overlaps partly the restricted superconductivity region with moderate  $T_c$  values. The pseudogap feature is currently known also for the electron doped systems [3-5,16,19,20]. There are some indications of presence of two pseudogaps connected with the quenching of the AF order by extended doping [4,20]. The pseudogap vanishes near the optimal doping distinguishable on the bell-like dependence of  $T_c$ . Decisive data on measured superconducting gaps in electron doped cuprates seem to be rare.

The pairing mechanism in cuprate high-temperature superconductors remains elusive. For this reason under a plenty of approaches a simple model basing on gross features known experimentally has been developed for description of hole doped cuprates [10,21,22]. On such a way one can presumably prove the general direction for elaborating a throughout theory and understand the nature of the pairing in cuprates. In the model mentioned the pairing interaction is supposed to be of interband nature between the itinerant and defect band states. There are numerous appointments that cuprate superconductors are multigap and multiband systems being recently supported by the direct measurement of two superconducting gaps in the LaSrCuO system [23].

The multiband superconductivity incorporating interband pairing is known for a long time [24,25]. It serves the simplest way to obtain high  $T_c$  values in the dispositions where several bands cross the Fermi surface and quantum resonance effects appear (for review see [26-28]). Recently the interest to multiband models in application to cuprates has essentially grown [32,34] stimulated also by the discovery of the multiband superconductor  $\text{MgB}_2$ . The model [19,21,22] describes self-consistently the behaviour of energetic [12,21,22], thermodynamic and other properties [29-31] of hole doped cuprates on the whole doping scale in qualitative agreement with the observations. The conception of the multicomponent nature of the cuprate superconductivity

[32] is supported by this.

In the present contribution an attempt to develop an analogous model for the electron doped cuprate superconductors is made.

## 2 The Model

The total number of states in the system including LHB, UHB and the defect band components supposed to be actual for the electron doped cuprate is normalized to one. The doped electron concentration for one Cu site and one spin will be denoted as  $c$ . According to [11] the UHB ( $\beta$ ) and LHB ( $\gamma$ ) weight of states under electron doping is  $(1/2 - c)$ . Note that this restricts the doping concentrations in our model to  $c < 1/2$ . The states exhausted from the Hubbard bands concentrate in the defect (midgap) band with the weight  $2c$ . The "itinerant" band densities are  $\rho_{\beta,\gamma} = (1/2 - c)/\Delta d$ , where  $\Delta d$  is the corresponding band width (2D case of  $\text{CuO}_2$  plane as superconductivity playground). Experimental data show that the functioning of momentum space regions around the  $(\pi, 0)$  and  $(\frac{\pi}{2}, \frac{\pi}{2})$  type points in the Brillouin zone must be differentiated near the Fermi energy, at least for underdoping. Therefore we introduce two defect subbands of weight  $c$  displaced in energy by  $d$ . The upper ( $\alpha 1$ ) corresponds to the  $(\pi, 0)$  neighbourhood, as also the  $\beta$ -band bottom (energy  $d_1$ ). The lower subband ( $\alpha 2$ ) corresponds to the  $(\frac{\pi}{2}, \frac{\pi}{2})$  neighbourhood. The  $\alpha 2$  band bottom is taken as energy zero.

The doping dependence of the pseudogap type excitations [4,6,19,20] and the build up of a common Fermi liquid at extended dopings suggest that the  $\alpha 1$  and  $\alpha 2$  top energies must evolve towards the  $\beta$ -band bottom. This is described by writing the corresponding energies as  $(d + \alpha c^2)$  and  $\alpha c^2$ . The quadratic dependence on concentration  $c$  has been suggested by the form of the pseudogap curves in [4,20]. The defect subbands densities  $\rho_\alpha(1, 2) = (\alpha c)^{-1}$  rise with doping and can be considered as determining a "flat band".

The  $(\alpha 1) - \beta$  gap closes with extended doping at the first critical point of the phase diagram with the concentration defined by  $c_0^2 = (d_1 - d)\alpha^{-1}$ . For  $c \leq c_0$  the chemical potential

$$\mu_1 = d + \alpha c^2 \quad (1)$$

remains connected with the upper defect subband  $\alpha 1$  (the  $\alpha 2$  component is filled). This agrees with the observation that at low dopings the electrons occupy the  $(\pi, 0)$  neighborhood which forms the Fermi surface pockets [5-7]. For  $c \geq c_0$  the  $\beta$  and  $\alpha 1$  bands overlap and become populated. Then

$$\mu_2 = (d + \alpha c^2 + d_1 \alpha c \rho_\beta)(1 + \alpha c \rho_\beta)^{-1}. \quad (2)$$

Two distinct (steep and flat) dispersions near  $(\pi, 0)$  have been measured in [6].

A further critical point  $c_x$  appears when  $\mu_2(c_x) = \alpha c_x^2$  and all the band components become intersected by the chemical potential. Such disposition is optimal for producing

maximal transition temperatures by the interband pairing mechanism. For  $c > c_x$

$$\mu_3 = (d + 2\alpha c^2 + d_1 \alpha c \rho_\beta)(2 + \alpha c \rho_\beta)^{-1}. \quad (3)$$

Accordingly a new spectral intensity around  $(\frac{\pi}{2}, \frac{\pi}{2})$  emerges, cf. [6,7]. The wider  $\beta$ -band contributes in the effective doping range to the formation of an electron-like Fermi surface. The chemical potential rises with electron doping in our model as stated in [2].

The central supposition of our approach is that the basic pairing channel consists in the pair transfer interaction [26] between the itinerant  $\beta$  and defect  $\alpha$ , 2 band states.

### 3 Superconductivity characteristics

We describe our superconducting system by the Hamiltonian

$$\begin{aligned} H = \sum_{\sigma, \vec{k}, s} \epsilon_\sigma(\vec{k}) a_{\sigma, \vec{k}, s}^+ a_{\sigma, \vec{k}, s} + \Delta_\beta \sum_{\vec{k}} [a_{\beta \vec{k} \uparrow} a_{\beta - \vec{k} \downarrow} + a_{\beta - \vec{k} \downarrow}^+ a_{\beta \vec{k} \uparrow}^+] \\ - \Delta_\alpha \sum_{\vec{k}, \alpha}^{1,2} [a_{\alpha \vec{k} \uparrow} a_{\alpha - \vec{k} \downarrow} + a_{\alpha - \vec{k} \downarrow}^+ a_{\alpha \vec{k} \uparrow}^+]. \end{aligned} \quad (4)$$

Here  $\epsilon_\sigma = \xi_\sigma - \mu$ ,  $\sigma = \alpha, \beta$ ,  $\sum_\alpha^{1,2}$  means the integration with the density ( $\rho_\gamma$ ) in the corresponding energy intervals for the defect bands. Usual designations for electron operators and spins ( $s$ ) apply. The superconductivity order parameters are defined as ( $\Delta_{\alpha, \beta} > 0$ )

$$\begin{aligned} \Delta_\beta &= 2W \sum_{\vec{k}, \alpha}^{1,2} \langle a_{\alpha \vec{k} \uparrow} a_{\alpha - \vec{k} \downarrow} \rangle, \\ \Delta_\alpha &= 2W \sum_{\vec{k}} \langle a_{\beta - \vec{k} \downarrow} a_{\beta \vec{k} \uparrow} \rangle. \end{aligned} \quad (5)$$

Here  $W > 0$  is the interband interaction constant. Its momentum dependence is neglected for simplicity, as also the contribution of intraband pairing channels.  $W$  is supposed to contain contributions of Coulomb (exchange) and electron-phonon nature [26].

The diagonalization of (1) yields the gap equation ( $\theta = k_B T$ ) system

$$\begin{aligned} \Delta_\beta &= W \Delta_\alpha \sum_{\vec{k}, \alpha}^{1,2} E_\alpha^{-1}(\vec{k}) \tanh \frac{E_\alpha(\vec{k})}{2\theta} \\ \Delta_\alpha &= W \Delta_\beta \sum_{\vec{k}} E_\beta^{-1}(\vec{k}) \tanh \frac{E_\beta(\vec{k})}{2\theta} \end{aligned} \quad (6)$$

with the quasiparticle energies

$$E_\sigma(\vec{k}) = \pm \sqrt{\epsilon_\sigma^2(\vec{k}) + \Delta_\sigma^2(\vec{k})} . \quad (7)$$

At  $T_c$  the superconductivity gaps  $\Delta_{\alpha,\beta}$  tend simultaneously to zero and one obtains from (5) an equation to calculate  $T_c$ . The condensation energy ( $H_{c0}^2/8\pi$ ) is represented by the thermodynamic critical field as

$$H_{c0} = \sqrt{4\pi[2\rho_\alpha\Delta_\alpha^2 + \rho_\beta\Delta_\beta^2]} . \quad (8)$$

Inspection of the minimal quasiparticle excitation energies explains the nature of the gaps expected to be observable in various doping windows [13].

## 4 The excitations

At heavy underdoping  $c < c_0$  the manifestation of two pseudogaps is expected in our model. The  $\beta$ -band connected pseudogap excitation energy equals (in the superconducting state)

$$\Delta_{p\beta} = [(d_1 - d - \alpha c^2)^2 + \Delta_\beta^2]^{1/2} \quad (9)$$

being minimal for quasiparticles of this band. The corresponding normal state gap ( $\Delta_\beta = 0$ ) closes at  $c_0$ . It determines the energy separation of occupied and empty states, being therefore an indicator of vanishing antiferromagnetic order. The second pseudogap is larger and corresponds to the  $\alpha 2$  band excitations in  $(\frac{\pi}{2}, \frac{\pi}{2})$  spectral window

$$\Delta_{p\alpha} = [d^2 + \Delta_\alpha^2]^{1/2} . \quad (10)$$

For  $c \geq c_0$  the pseudogap  $\Delta_{p\beta}$  vanishes transforming into the  $\beta$ -band superconducting gap. It determines now the minimal quasiparticle excitation energy of this band. The smaller pseudogap continues at  $c > c_0$  with stronger doping dependence as

$$\Delta_{p\alpha} = [(\mu_2 - \alpha c^2)^2 + \Delta_\alpha^2]^{1/2} . \quad (11)$$

The superconducting gap  $\Delta_\alpha$  can be discovered at this in the  $(\pi, 0)$  type window (the  $\alpha 1$  band encloses  $\mu$ ).

The normal state gap corresponding to  $\Delta_{p\alpha}$  closes at  $c_x$ . Beyond  $c_x$  the excitation spectrum is expected to be determined by both superconducting gaps  $\Delta_\beta$  and  $\Delta_\alpha$ . The latter must now be detectable in the whole momentum window. With vanishing  $\Delta_{p\alpha}$  at  $c_x$  in the normal state the tracks of AF ordering vanish at all. Note that the pseudogaps appear in our model as precursors of superconducting gaps on the doping, but not on the energetic (phase diagram vertical) scale. The pseudogap vanishes, i.e. transforms to superconducting gap in effectively or overdoped samples as observed [4,6,19,20]. However the normal state gaps can enter the superconducting energy domain before

reaching zero. At critical point where the pseudogap closes an insulator-metal crossover is expected in the normal state. Such transition has been observed experimentally [33]. And moreover – the characteristic resistivity temperature *vs* curve seems to follow the pseudogap doping dependence.

## 5 Illustrative results

A seemingly plausible parameter set has been chosen to illustrate the outcome of the presented model for a "typical" electron-doped cuprate superconductor. A maximal value of  $T_c$  round 30 K near  $c = 0.15$  in the superconductivity domain extending from  $c = 0.07$  until  $c = 0.3$  has given experimental guidance. The numerical calculations have been made taking  $d = 0.03$ ;  $d_1 = 0.1$ ;  $\Delta d = 1.0$  and  $\alpha = 10$  (eV). The interband coupling constant  $W = 0.175$  eV leads then to  $T_{cm} = 28$  K at  $c = 0.15$ . The critical electron doping concentrations read at this  $c_0 = 0.08$  and  $c_x = 0.13$ .

In Figure 1 the dependence of transition temperature, chemical potential and normal state (pseudo) gaps on doping are shown. Remarkable values of  $T_c$  are reached first near  $c_0$  where two overlapping bands enter into resonance with  $\mu$ . The maximal  $T_c$  is reached when the resonance of all three band components have somewhat deepened beyond  $c_x$ . Concerning the absolute value of  $T_c$ , the present model states that electron doping of the strongly correlated system cannot proceed too far ( $c < 0.5$ ) without a collapse of the basic spectrum. Extended doping leads to quenching of the whole interband machinery. One sees in Fig.1 that the smaller pseudogap can enter the superconductivity domain. For the behavior of the pseudogaps cf. Fig.1 in [4] where the smaller one is given under the question mark. The present model predicts the presence of this second pseudogap.

In Figure 2 the calculated ( $T = 0$ ) superconductivity gaps and the condensation energy ( $H_{c0}$ ) on the doping scale are given.

Figure 3 illustrates the behavior of excitation gaps in the superconducting state at  $T = 0$ . One can see the transformation of the larger pseudogap into the UHB  $\beta$ -superconducting gap  $\Delta_\beta$  at  $c_0$ . For  $c < c_0$  the contribution of  $\Delta_\beta$  is hidden in the  $\Delta_{p\beta}$ . The same happens with the smaller pseudogap and the defect superconducting gap  $\Delta_\alpha$  in the  $(\frac{\pi}{2}, \frac{\pi}{2})$  window. Note that at  $c < c_x$  the gap  $\Delta_\alpha$  (see the fragment of it in Fig.2) must be detectable in the  $(\pi, 0)$  window. At  $c > c_x$   $\Delta_\alpha$  must be observable in both windows as seen in Fig.2. The energy scales of the pseudo- and superconducting gaps can be comparable out of the underdoped region. This can prepare difficulties when interpreting fragmental data of measurements. In analyzing the manifestations of two spectral gaps there can arise problems because the states associated with the smaller gap can mask the sharpness of the larger gap. The peak associated with the latter can then appear as a spectral hump, cf. [6]. The characteristic gap relations  $2\Delta_{\alpha,\beta}/kT_c$  violate the BCS universality and does not change markedly with doping being about

4.8 for the  $\beta$  and 2.6 for the  $\alpha$  band. The condensation energy given also in Fig.2, shows the usual bell-like dependence.

As a result it seems that the present model is able to explain the gross nature of the electron-doped cuprate phase diagram. Detailed investigations of the number of pseudogaps and on the superconducting gaps in the whole doping region in a single experiment were of considerable interest to prove some of our conclusions looking as predictions.

At present one can seemingly constatate that in both cases of hole and electron doped cuprate superconductors the deepest background is the same. The necessary doping metallizes the basic strongly correlated materials and prepares transformed electron structures with new energetic states. However, these novel backgrounds having comparable elements and functioning are realized in different manner and on different sublattices. In the case of electron doping it is the Cu-sublattice and doping influences immediately the spectrum built by strong electron correlations. In the case of hole doping it is the highly polarizable and deformable oxygen sublattice. The universal multiband pairing mechanism leads in both cases to the comparable characteristic phase diagrams of high-temperature superconductivity.

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Fig.1. The transition temperature (1), chemical potential (2), the large (3) and small (4) normal state (pseudo)gaps of a cuprate on the electron doping (c) scale.

Fig.2. The calculated zero temperature superconducting gaps and the thermodynamic critical field representing the condensation energy  $H_{co}^2(8\pi)^{-1}$ .

Fig. 3. The excitation energies represented by the pseudogap and superconducting components on the electron doping scale ( $T = 0$ ). 1 -  $\Delta_{p\alpha}$  and  $\Delta_{\alpha}$ ; 2 -  $\Delta_{p\beta}$  and  $\Delta_{\beta}$ .



## References

- [1] A.Damascelli, Z.Hussain, Z.-X-Shen, Rev. Mod. Phys. **75**, (2003) 473.
- [2] N.Harima et al., Phys. Rev. B **64**, (2001) 220507R.
- [3] A.Biswas et al., Phys. Rev. B **64**, (2001) 104519.
- [4] L.Alff et al., Nature **422**, (2003) 698.
- [5] T.Tohyama, Physica C **412-414**, (2004) 139.
- [6] H.Matsui et al., Phys. Rev. Lett. **94**, (2005) 047005.
- [7] S.R.Park et al., Phys. Rev. B **75**, (2007) 060501R.
- [8] S.Uchida et al., Phys. Rev. **43** (1991) 7942.
- [9] M.Tachiki, in: *Strong Correlation and Superconductivity*, edited by H.Fukuyama et al. (Springer, Berlin, 1989) p. 139.
- [10] T.Takahashi, Physica C **170**, (1990) 416.
- [11] M.B.J.Meinders, H.Eskes, G.A.Sawatzky, Phys. Rev. **48**, (1993) 3916.
- [12] N.Kristoffel, P.Rubin, in *Symmetry and Heterogeneity in High-Temperature Superconductors*, edited by A.Bianconi (Springer, 2006) p.55.
- [13] N.Kristoffel, P.Rubin, Solid State Commun. **122**, (2002) 265.
- [14] *Phase separation in cuprate superconductors*, edited by K.A.Müller and G.Benedek (World Sci., Singapore 1993).
- [15] C.Kusko et al., Phys. Rev. B **66**, (2002) 140513(R).
- [16] Q.Yuan, X.-Z.Yan, C.S.Ting, Phys. Rev. B **74**, (2006) 215403.
- [17] B.Kyung et al., Phys. Rev. Lett. **93**, (2004) 147004.
- [18] D.K.Sunko, S.Barisic, Phys. Rev. B **75**, (2007) 060506(R).
- [19] N.P.Armitage, Phys. Rev. Lett. **87**, (2001) 147003.
- [20] Y.Onose et al., Phys. Rev. Lett. **87**, (2001) 217001.
- [21] N.Kristoffel, P.Rubin, Physica C **402**, (2004) 257.
- [22] N.Kristoffel, P.Rubin, J. Supercond. **18**, (2005) 705.

- [23] R.Khasanov et al., Phys. Rev. Lett. **98**, (2007) 057007.
- [24] H.Suhl, B.T.Matthias, L.R.Walker, Phys. Rev. Lett. **3**, (1959) 552.
- [25] V.A.Moskalenko, Fiz. Met. Metalloved. **8**, (1959) 503.
- [26] N.Kristoffel, P.Konsin, T.Örd, Rivista Nuovo Cim. **17**, (1994) 17.
- [27] A.Bianconi, J. Supercond. **18**, (2005) 25.
- [28] A.Bianconi, M.Filippi, in: *Symmetry and Heterogeneity in High-Temperature Superconductors*, edited by A.Bianconi (Springer, 2006) p. 21.
- [29] N.Kristoffel, T.Örd, P.Rubin, Physica C **437-438**, (2006) 168.
- [30] N.Kristoffel, P.Rubin, Phys. Lett. A **356**, (2006) 249; *ibid.* **360**, (2006) 367.
- [31] N.Kristoffel, T.Örd, P.Rubin, in *Electron Correlation in New Materials and Nanosystems*, edited by K.Scharnberg and S.Kruchinin (Springer, 2007) p. 275.
- [32] K.A.Müller, Physica C **341-348**, (2000) 11.
- [33] P.Fournier et al. Phys. Rev. Lett. **81**, (1998) 4720.





